

Citation: Eschenroeder, A., M. Lorber. 1999. An Evaluation of EPA's ISCST - Version 3 model Part 1. Air dispersion of dioxins. Presented at Dioxin '99, the 19th International Symposium on Halogenated Environmental Organic Pollutants and POPs, held September 12-17 in Venice, Italy. Short paper in, *Organohalogen Compounds*, Volume 41:547-552.

Posting of short paper approved by Ecoinforma Press, Jean-Paul-Str. 30, D-95444 Bayreuth.  
Fax: 49-021-54626. E-Mail: [otto.hutzinger@uni-bayreuth.de](mailto:otto.hutzinger@uni-bayreuth.de)

## **An Evaluation of EPA's ISCST -Version 3 Model**

### **Part 1. Air Dispersion of Dioxins**

Alan Eschenroeder<sup>1</sup>, Matthew Lorber<sup>2</sup>

<sup>1</sup>Harvard School of Public Health, Department of Environmental Health, Boston, MA; <sup>2</sup>National Center for Environmental Assessment (8623D), United States EPA, Washington, DC 20460

#### **Introduction**

The central purpose of our study is to examine the performance of the United States Environmental Protection Agency's (US EPA) nonreactive Gaussian air quality dispersion model, the Industrial Source Complex Short Term Model (ISCST3) Version 98226, in predicting polychlorinated dibenzodioxins and polychlorinated dibenzofurans concentrations (subsequently referred to as dioxins and furans, or CDD/Fs) near the Columbus Municipal Waste-to-Energy Facility (CMWTE) in Columbus, Ohio. The plant operated between June 1983 and December 1994 and was estimated to emit nearly a kilogram of dioxin toxic equivalents (TEQs) annually (TEQs calculated in this paper use the International TEF scheme<sup>1</sup> and do not include dioxin-like PCBs). This compares with US estimates of total emissions of 12 kg TEQ in 1987 and 3 kg in 1995<sup>2</sup>. Two 48-hour measurement periods, March 17 – 19, 1994 and April 19 – 21, 1994, provide time-averaged ambient concentrations at six monitoring stations of the 17 individual 2,3,7,8 congeners as well as those of the 8 homologue groups. A third 48-hour measurement period, from May 30 to June 1, 1995 at the same six stations, occurred after the CMWTE had shut down. During the same 48-hour period of the March 17-19 ambient air monitoring event, stack emissions of dioxins from the CMWTE were measured. This stack measurement and the air measurements in 1994 and 1995, combined with concurrently measured meteorological data, provide the basis for the model evaluation exercises described here. Complete descriptions of the measurement and analysis programs conducted around this facility are available in previous papers<sup>3,4,5</sup> and not repeated here.

#### **Modeling procedures**

ISCST3 is a Gaussian plume model, which accepts a variety of source geometries and emissions schedules in order to compute ambient air concentrations and surface deposition fluxes at specified receptor points. The short term version of the model used here relies on hourly wind

speed, wind direction and stability for describing dispersion. Rainfall data is required for deposition, but no rain fell on either 1994 sampling date. Also, the air dispersion algorithms alone were tested in this paper, so no rainfall data was required to run ISCST3. The dioxins were modeled as if the entire emission were in the form of a conservative pollutant, a simplification chosen here for ease of model testing. Besides meteorological data, other required inputs include: (1) building configuration data, (2) emissions data, and (3) receptor data. Due to space considerations, details on parameter assignments for this modeling exercise cannot be provided in this abstract. Further detail on the ISCST3 can be found in EPA<sup>6</sup>.

The ISCST3 model computed unit ambient concentrations, i.e., concentrations at receptor points assuming a one gram per second emission rate. The individual total emission rates of each CDD/F multiplied by the unit concentration gave the ambient concentrations at the receptor points. The stack test conducted in March 1994<sup>7</sup> during the ambient air sampling event gave a TEQ emission rate of  $7.9 \times 10^{-6}$  g/sec (250 g TEQ/yr). This stack test was conducted after measures were taken to specifically reduce dioxin emissions; a previous test conducted in 1992<sup>8</sup> suggested emissions fourfold higher at 976 g TEQ/yr.

Two sets of meteorological data are used in this study: an "airport" set and an "on-site" set. The airport set includes surface data (wind speed, wind direction and atmospheric stability) from the Columbus, Ohio airport and upper air data for the mixing height from Dayton, Ohio airport<sup>9</sup>. On-site data for both of the 1994 measurement periods<sup>10</sup> include wind speed and wind direction. The Columbus stability and Dayton mixing height were used in the on-site set.

Analyses of on-site wind roses for the March and April 1994 sampling dates reveal that there is one dioxin monitoring station likely to have been influenced by the CMWTE. This station, termed SE-3 by the Ohio Environmental Protection Agency (OEPA)<sup>3,4</sup> was about 2 km east of the source and was downwind from the source approximately 53% of the time during the sampling period in March 1994 and 78% of the time in April 1994<sup>3</sup>. In contrast, none of the other 5 stations was downwind for time fractions approaching those of SE-3. The measurements confirmed that SE-3 was the most impacted of the samplers, with TEQ measurements of 168 fg TEQ/m<sup>3</sup> in March and 353 fg TEQ/m<sup>3</sup> in April. The average of the measurements from the other 5 samplers over the two dates (a total of 8 samples; one sampler was not operational for both events) was 52 fg TEQ/m<sup>3</sup>, with a range of 10 to 98 fg TEQ/m<sup>3</sup>. Lorber<sup>5</sup> examined this trend further, showing also that the profile of CDD/Fs found in March and April in SE-3 matched the stack emission profile of CDD/Fs much more closely than the other ambient air samples, which displayed profiles more typical of background air.

To isolate the effect of the source, background concentrations were subtracted from the measurements. The average of 6 air measurements taken in 1995 after the CMWTE shut down was assumed to represent the background dioxin air concentrations for this site. The average total concentration from 1995 was 2870 fg/m<sup>3</sup>, with a range of 2030 to 4760 fg/m<sup>3</sup>. "Total concentrations" are defined as the sum of homologue group concentrations in this paper. The 1995 average concentrations of each 2,3,7,8-substituted congener as well as those of the homologue groups were subtracted from each of the March and April 1994 corresponding measurements. When such a subtraction resulted in a concentration less than 0, the concentration was assumed to be 0 for purposes of this exercise.

## Results

Table 1 compares the observed total concentrations at each reporting monitoring station with the

model predictions for both meteorological data sets, the “on-site” and “airport” sets. While ISCST3 can predict short-term air concentrations, its recommended use is principally to predict annual average concentrations from running simulations on one or more years of meteorological data. Therefore, the paired comparisons of predicted and observed 48-hr air concentrations are severe tests of model performance, and Table 1 shows the large scatter expected from this test.

Still, some meaningful observations might be possible. First, it does appear as if model runs using the on-site meteorological data better duplicated the field observations compared to model runs using the airport data: the correlation between observed and predicted was 0.57 with the on-site data and 0.12 with the airport data, combining March and April results. The slope of the best-fit regression lines also favors the on-site data: it was 0.77 for on-site versus 0.21 for airport. This comparison shows the importance of using on-site meteorological data for short-term model/measurement comparisons.

Additionally, it might be reasonable to observe that the on-site model results generally followed the trend in 7 of 9 March/April measurements - that is, predicted air concentrations were negligible when the measured air concentrations were low, and high air concentrations were predicted when they occurred. However, the model predicted meaningful impacts where none were measured for SNW-1 in March and SSW-4 in April. There appeared to be some overprediction in March but underprediction in April. The underprediction in April could be due to the use of the March stack test to represent emissions for the April sampling event - it is possible that more dioxin was emitted from the CMWTE during April as compared to March.

As mentioned above, station SE-3 stands out in both the March and April sampling as having the highest impact of all stations. Thus, the data from this station have the best chance of avoiding the uncertainties introduced by background fluctuations. Predicted and observed homologue group concentrations for SE-2 for the both sampling dates are compared in Table 2. These results were generated using on-site meteorological data. Table 2 also shows the CMWTE stack emission rate of these homologue groups.

Being only an exercise in air dispersion modeling (no wet/dry deposition; no stack speciation), it is easy to see the expected perfect correlation between the homologue profile of the emissions and air concentration predictions for both March and April. The observed air concentrations clearly do not have this stack emission profile, however, and the subsequent correlation between predicted and observed is low: 0.36 for March and April combined. The speciation pattern from source to receptor has shifted in these ways: 1) the lower chlorinated tetra and penta CDD/Fs have greatly magnified in importance in the ambient air profile as compared to the stack profile, and 2) conversely, the hexa through octa homologues, with the exception of OCDF, have been reduced in importance in the ambient air profile as compared to the stack profile. The model predicted lower concentrations for the lower chlorinated CDD/Fs than were measured, and higher concentrations for the higher chlorinated CDD/Fs. The total concentration predictions were, however, within about a factor of two of observations. Not that it has meaning with regard to fate and transport considerations, but the TEQ concentrations were comparable: 125 and 309 fg TEQ/m<sup>3</sup> measured during March and April compared with 135 and 130 fg TEQ/m<sup>3</sup> modeled for SE-3.

Three possible explanations are offered to explain why the model did not predict the measured shift in homologue profile between the stack and field:

- 1) It is known that CDD/Fs with fewer chlorines have higher vapor to particle (V/P) ratios<sup>11</sup>; indeed, high temperatures in the stack generate even higher V/P ratios<sup>12</sup>. If stack

sampling methods underestimate the amount of vapor pollutant being emitted, than the lower chlorinated dioxin emission rates are being underestimated - an error that would be exacerbated by the even higher V/P ratios in the high temperature stack gas. The PS-1 samplers capturing both vapor and particle-phase CDD/Fs in ambient air are well tested and not expected to have caused error in ambient air sampling.

2) Running the air dispersion algorithms of ISCST3 alone did not account for particle deposition, yet some of the higher chlorinated CDD/Fs, expected to be sorbed to ambient air particles or fly ash, may have deposited by dry deposition prior to the air sampling locations. The companion paper to this one<sup>13</sup> supports this hypothesis, at least for the dioxins. It compares model predictions of soil concentration with measured soil concentrations. One clear trend was that the model consistently underpredicted the soil concentration of the hepta and octa dioxin homologue groups. This result, combined with the observation that the higher chlorinated dioxins were the most overpredicted in air concentrations in this paper, suggests that the plume is being depleted of higher chlorinated dioxins by deposition. However, this trend was not duplicated by the higher chlorinated furans. There, modeled soil concentrations were more nearly consistent with measured soil concentrations, with a small degree of overprediction.

3) Another possible physical explanation is that dechlorination may occur between the emission point and the ambient measuring station a kilometer or two downwind. Workers at Monsanto Laboratories<sup>14</sup> and at the Agro-Environmental Science Institute in Japan<sup>15</sup> have observed photolysis of TCDD. Generally, polychlorinated organic compounds easily experience photochemical loss of chlorine atoms. If the higher chlorinated CDD/Fs dechlorinated to form lower chlorinated CDD/Fs in the atmosphere, than more lower chlorinated CDD/Fs would have arrived at the ambient air monitoring stations to cause the distinct ambient air profile.

### **Concluding remarks**

While admittedly a limited field test of an air dispersion model, the data used here had these important features, which are not readily (if at all) available for similar model testing: a stack test taken at the same time surrounding air quality was monitored, a very high release rate of dioxins such that a signal could easily be identified in the air monitors, on-site meteorological data taken at the time of stack and ambient air testing, and data available to distinguish the background from a "signal" of dioxin in the measured data. The air dispersion modeling done here suggests that predicted air concentrations of CDD/Fs are within a factor of 10 of observations, and mostly within a factor of 5 of observations. Follow-up modeling exercises will test if particle deposition or photolytic dechlorination could account for the observed homologue shift between the stack and field. While the analysis in this paper as well as the companion paper on deposition/soil concentration modeling<sup>13</sup> are not intended as rigorous model evaluations, they will hopefully stimulate interest in conducting coordinated model runs, source tests and field ambient measurements to better understand the processes that may influence the fate and transport of dioxins emitted from tall stacks.

### **References**

1. US EPA. Interim procedures for estimating risks associated with exposures to mixtures of chlorinated dibenzo--p-dioxins and -dibenzofurans (CDDs and CDFs) and the 1989 Update. Risk Assessment Forum, Washington, DC; EPA/625/3-89/016. **1989**.

2. Cleverly, D; Schaum, J; Winters, D; Schweer, G.; O'Rourke, K. **1998**, *Organohalogen Compounds*, 36, 1.
3. Ohio EPA *Franklin County Ambient Air Monitoring Study for Dioxins and Dibenzofurans*. July, **1994**.
4. Ohio EPA. *Dioxin Monitoring Study 1995 Franklin County, Ohio*. September, **1995**.
5. Lorber, M; Pinsky, P; Gehring, P; Braverman, C; Winters, D; Sovocool, W. **1998**, *Chemosphere*, 37, 2173.
6. USEPA, *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Vol I – User Instructions and Vol II–Description of Model Algorithms*, **1995**. EPA-454/B-95-003a,b.
7. EMC Analytical, Inc. Emission Study Performed for Solid Waste Authority of Central Ohio, Project No: 35001, April 18, **1994**.
8. Energy and Environmental Research Corporation. Permit Compliance Test Report, Columbus Solid Waste Reduction Facility. Submitted to: Ohio EPA, September 11, **1992**.  
BEEline Software, Inc. ISCST3 driver diskette **1998**  
Ohio Environmental Protection Agency. private communication **1998**
11. Bidleman, T.F. *Environ. Sci. and Tech.*, **1988**, 22, 361.
12. Eschenroeder, A., Cullen, A. C; von Stackelberg, K. *Gas/Particle Partitioning effects on Dioxin Exposures from Incinerators*, a paper presented at the U.S. Environmental Protection Agency Ninth Annual Regional Risk Assessment Conference, April 25-27, **1994**.
13. Lorber, M; Eschenroeder, A.; Robinson, R.; An Evaluation of EPA's ISCST -Version 3 Model Part 2. Deposition and Soil Concentration of Dioxins. This conference.
14. Orth, R.O.; Ritchie, C; Hileman, F., *Chemosphere* , **1987**, 18, p 1275.
15. Koshioka, M.; Yamada, T; Knazawa, J; Murai, T. *Chemosphere*, **1989**, 19, 681.

**Table 1.** Comparison of observed and modeled total CDD/F concentration increments at the urban monitoring stations (total = sum of homologue group concentrations; on-site, airport = model results generated using on-site and airport meteorological data).

| Station | March 94 Sampling, fg/m <sup>3</sup> |         |         | April 94 Sampling, fg/m <sup>3</sup> |         |         |
|---------|--------------------------------------|---------|---------|--------------------------------------|---------|---------|
|         | Observed                             | On-site | Airport | Observed                             | On-site | Airport |
| SN-2    | 1321                                 | 1778    | 3598    | 0                                    | 0       | 0       |
| SE-3    | 6368                                 | 7808    | 2912    | 16105                                | 7557    | 1161    |
| SNW-1   | 0                                    | 7968    | 1326    | 557                                  | 0       | 0       |
| SSW-4   | 0                                    | 0       | 0       | 3682                                 | 7598    | 9536    |
| HSCNE   | NA                                   | NA      | NA      | 1493                                 | 123     | 64      |

**Table 2.** Comparison of observed and modeled homologue and TEQ concentrations at station SE-3 using on-site meteorological data for model input.

| Homologue Group | Stack Emission Rate, ng/dscm | SE - 3, March 94, fg/m <sup>3</sup> |             | SE - 3, April 94, fg/m <sup>3</sup> |             |
|-----------------|------------------------------|-------------------------------------|-------------|-------------------------------------|-------------|
|                 |                              | Observed                            | Modeled     | Observed                            | Modeled     |
| TCDD            | 32                           | 490                                 | 67          | 851                                 | 65          |
| PCDD            | 97                           | 594                                 | 204         | 1144                                | 198         |
| HxCDD           | 300                          | 543                                 | 632         | 1402                                | 611         |
| HpCDD           | 508                          | 424                                 | 1078        | 1378                                | 1043        |
| OCDD            | 578                          | 384                                 | 1225        | 1575                                | 1185        |
| TCDF            | 293                          | 904                                 | 624         | 1976                                | 604         |
| PCDF            | 439                          | 1226                                | 934         | 2982                                | 904         |
| HxCDF           | 648                          | 951                                 | 1370        | 2518                                | 1326        |
| HpCDF           | 616                          | 718                                 | 1300        | 1846                                | 1258        |
| OCDF            | 170                          | 134                                 | 375         | 433                                 | 362         |
| <b>Total</b>    | <b>3681</b>                  | <b>6368</b>                         | <b>7809</b> | <b>16105</b>                        | <b>7557</b> |
| <b>TEQ</b>      | <b>64</b>                    | <b>125</b>                          | <b>135</b>  | <b>309</b>                          | <b>130</b>  |